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ENERGY AND SOME ATOMIC PROPERTIES FOR EXCITED STATE OF AR^{+16} ION USING HARTREE-FOCK METHOD

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ABSTRACT

Expectation values of energies (potential, kinetic, Hartree-Fock, repulsion and attraction)forAr^{+16}ion in some excited state (1sns) where n=2,3,4,5 had been studied using " two-electron density function Γ (r_1,r_2)" to analyze Hartree-Fock equations using "slater type orbitals" also we calculated " nuclear magnetic shielding constant σ_d" and "the diamagnetic susceptibility x_d" of this excited state for Ar^{+16}.

KEYWORDS: Hartree-Fock Method, Two Electron Density Function, Slater Type Orbitals, The Diamagnetic Susceptibility & The Nuclear Magnetic Shielding Constant

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Original Article

INTRODUCTION

The hartree-Fock method is one of an approximated method for calculation ground state and excited states wave functions of multi-electron systems and it is a convenient method for studying of the electronic structure of atoms and molecules in this work, radial part of basis function is" slater type orbital (STO) " which defined as [1]

$$\chi_{nlm_l}(\xi, r) = (2\xi)^{n+\frac{1}{2}}[(2n)!]^{-\frac{1}{2}}\, r^{n-1}\exp(-\xi r)Y_{lm_l}(\theta, \phi) \tag{1}$$

Where, ξ_i> 0 is the "orbital exponent".(n) a" positive principal quantum number of (STO)",$Y_{lm}(\theta, \phi)$ is a" spherical harmonic".

THEORY

By using "two-particle density matrix"$\Gamma(x_m, x_n)$,we can calculate physical properties of electronic structure of multi electron systems instead of using wave function $\psi(x_1, x_2, \dots . x_N)$ because "two-particle density matrix"$\Gamma(x_m, x_n)$ include all the important information properties to compute many properties and energy of multi electron systems. "two-particle density matrix"$\Gamma(x_m, x_n)$ defined as [2]

$$\Gamma(x_1, x_2) = \frac{N(N-1)}{2}\int \dots \int |\psi(x_1, x_2, \dots . x_N)\,|^2\, dx_3 \dots . dx_N \tag{2}$$

Where x_i=(r_i, s_i) space and spin variable which

s = α(spin up)and β(spin down). $\Gamma(x_1, x_2)$ gives the probability that one electron will be found at x_1 and another electron will be found at x_2 of N electrons.$\frac{N(N-1)}{2}$ represent number of electron pairs.

Expectation Values of Energy

The expectation value of energy $\langle E\rangle$ is given by [3]

$$\langle E\rangle = \langle T\rangle + \langle V\rangle \quad (3)$$

Where $\langle T\rangle$ is the kinetic energy and $\langle V\rangle$is the potential energy which given by [4]

$$\langle V\rangle = \langle V_{en}\rangle + \langle V_{ee}\rangle \quad (4)$$

Where $\langle V_{en}\rangle$ is the attraction energy between an electron and nucleuswhich defined by [5].

$$\langle V_{en}\rangle = -Z.\langle r_1^{-1}\rangle \quad (5)$$

$$\langle V_{ee}\rangle = \langle r_{12}^{-1}\rangle \quad (6)$$

Which$\langle r_1^{-1}\rangle$ represents "one electron expectation value" and it is determined by [6]

$$\langle r_1^m\rangle = \int_0^\infty D(r_1) r_1^m \, dr_1 \quad (7)$$

m is integer number,r_1 is the distance between an electron and nucleus, $D(r_1)$represents "one-electron radial density function" given by [7]

$$D(r_1) = \int_0^\infty D(r_1, r_2) dr_2 \quad (8)$$

Where $D(r_1, r_2)$ represents "two electron radial density function" defined by

$$D(r_1, r_2) = \iint \square(r_1, r_2) r_1^2 r_2^2 \, ds_1 ds_2 d\Omega_1 d\Omega_2 \quad (9)$$

$$d\Omega_i = \sin\theta_i d\theta_i \, d\emptyset_i$$

Ω_i is the solid angle, $\langle V_{ee}\rangle$ is repulsion energy between electron-electron

$\langle r_{12}^{-1}\rangle$ represents"inter particle expectation value" given by the relation

$$\langle r_{12}^{n}\rangle = \int_0^\infty f(r_{12}) r_{12}^{m} \, dr_{12} \quad (10)$$

$f(r_{12})$ is a "radial electron-electron distribution function" and r_{12} is the distance between two-electrons

"Nuclear Magnetic Shielding Constant"σ_d

"Nuclear magnetic shielding constant"is determined by the relation [8].

$$\sigma_d = \frac{1}{3} \acute{\alpha}^2 \langle \psi | \sum_{i=1}^{n} (r_i)^{-1} | \psi \rangle \quad (11)$$

($\acute{\alpha}$) is the fine structure constant $\acute{\alpha} = \frac{1}{c}$

The Diamagnetic Susceptibility x_d

The Diamagnetic Susceptibility is given by the relation [9]

$$\chi_d = {-\langle r^2\rangle}/{(6c^2)} \quad (12)$$

Where (c) is the speed of light in atomic units

RESULT AND DISCUSSIONS

Using Hartree-Fock wave function, Ar^{+16}ion had been studied in its excited states (1sns) where n=2,3,4,5. This system consists of two electrons one electron in K-shell (1S) state and another electron in (nS) state in shells (L,M,N,O) shells. It was calculated expectation value of potential energy $\langle V\rangle$, expectation values of kinetic energy $\langle T\rangle$, expectation values of repulsion energy $\langle V_{ee}\rangle$, expectation values of attraction energy $\langle V_{en}\rangle$ and expectation values of Hartree-Fock energy<E>. Also, it was computed some atomic properties for this system such as" nuclear magnetic shielding constant" σ_d and "the diamagnetic susceptibility x_d".

Table (1) lists some expectation values of energies (potential $\langle V\rangle$, kinetic $\langle T\rangle$, repulsion $\langle V_{ee}\rangle$, attraction $\langle V_{en}\rangle$ and Hartree-Fock<E>) in (1sns) state for Ar^{+16}ion. Table (2) shows some calculated values of " nuclear magnetic shielding constant $\boldsymbol{\sigma_d}$" for Ar^{+16} ion. Table (3) represents some computed values of "the diamagnetic susceptibility $\mathbf{x_d}$" for Ar^{+16} in (1sns) state. All result in atomic unit.

Table 1: Expectation Values of (Potential Energy $\langle V\rangle$, Kinetic Energy $\langle T\rangle$, Hartree-Fock Energy<E>, Repulsion Energy $\langle V_{ee}\rangle$ and Attraction Energy $\langle V_{en}\rangle$ for Ar^{+16} Ion in its Excited State

State				$-\langle V_{en}\rangle$for 1s	$-\langle V_{en}\rangle$for ns
1s 2s	-398.097997	-199.04899	3.38183	339.894	61.6082
1s 3s	-356.5632	-178.281598	1.67852	327.672	30.5659
1s 4s	-342.24041	-171.12021	0.97958	325.404	17.8125
1s 5s	-335.64831	-167.82416	0.63885	324.6876	11.5994

Table 2: Nuclear Magnetic Shielding Constant for Ar^{+16} in (1sns) State

State	σ_d x10^{-5}
1s 2s	6.07541
1s 3s	3.01421
1s 4s	1.75656
1s 5s	1.14386

Table 3: Diamagnetic Susceptibility x_d for Ar^{+16} in Different Excited State

State	χ_d x 10^{-6}
1s 2s	- 1.21095
1s 3s	-6.14463
1s 4s	-19.4698
1s 5s	-47.5851

CONCLUSIONS

This paper studied Ar^{+16} in some excited states (1s2s,1s3s,1s4s,1s5s) ^{1}s state and calculated expectation values for (potential, kinetic, Hartree-Fock, repulsion, and attraction)energies. Also in this study we examined and calculated "nuclear magnetic shielding constantσ_d" and "the diamagnetic susceptibilityx_d" for this system using MathCAD 2001i program and all result was in the atomic unit.

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